United States
Environmental Protection Agency

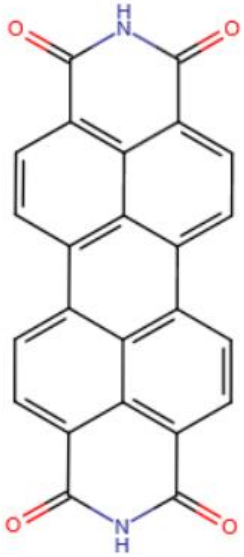
Office of Chemical Safety and
Pollution Prevention

# Final Risk Evaluation for C.I. Pigment Violet 29 (Anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone)

## Systematic Review Supplemental File:

## Data Quality Evaluation of Environmental Fate and Transport Studies

## CASRN: 81-33-4




*January 2021*

This document is a compilation of tables for the data extraction and evaluation for C.I. Pigment Violet 29 (CASRN 81-33-4). Each table shows the data point or set or information element that was extracted and evaluated from a data source in accordance with Appendix D of the *Application of Systematic Review in TSCA Risk Evaluations* (U.S. EPA (2018). If the source contains more than one data set or information element, the review provides an overall confidence score for each data set or information element that is found in the source. Therefore, it is possible that a source may have more than one overall quality/confidence score.

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**Table 1. EPI Suite™ Modeling Program, U.S. EPA (2012)**

| Study Reference: | U.S. EPA Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. 2012. | | | | | |
|---|---|---|---|---|---|---|
| **Domain** | **Metric** | **Qualitative Determination [*i.e.*, High, Medium, Low, Unacceptable, or Not rated]** | **Comments** | **Metric Score** | **Metric Weighting Factor** | **Weighted Score** |
| **Test Substance** | 1. Test substance identity | High | The test substance was identified by chemical structure. | 1 | 2 | 2 |
| | 2. Test substance purity | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Test Design** | 3. Study Controls | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 4. Test Substance stability | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Test Conditions** | 5. Test Method Suitability | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 6. Testing Conditions | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 7. Testing Consistency | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 8. System Type and Design | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Test Organisms** | 9. Test Organism Degradation | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 10. Test Organism Partitioning | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Outcome Assessment** | 11. Outcome Assessment Methodology | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 12. Sampling Methods | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Confounding/ Variable Control** | 13. Confounding Variables | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 14. Outcomes | Not rated | The metric is not | NR | NR | NR |

| Study Reference: | U.S. EPA Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. 2012. | | | | | |
|---|---|---|---|---|---|---|
| | Unrelated to Exposure | | applicable to this study type (SAR). | | | |
| **Data Presentation and Analysis** | 15. Data Reporting | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 16. Statistical Methods and Kinetic Calculations | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| **Other** | 17. Verification or Plausibility of Results | Not rated | The metric is not applicable to this study type (SAR). | NR | NR | NR |
| | 18. QSAR Models | High | The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r2, q2) for the regressions of some environmental fate models (*i.e.*, BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient). | 1 | 1 | 1 |
| | | | **Sum of scores:** | 2 | 3 | 3 |
| High | Medium | Low | **Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:** | 1 | **Overall Score (Rounded):** | 1 |

| Study Reference: | U.S. EPA Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. 2012. | | | | | |
|---|---|---|---|---|---|---|
| ≥1 and <1.7 | ≥1.7 and <2.3 | ≥2.3 and ≤3 | | | **Overall Quality Level:** | High |
| Note: The reviewer agreed with this study's overall quality level. | | | | | | |

**Table 2. Activated Sludge Study for C.I. Pigment Violet 29, BASF (1999b)**

| **Study Reference:** | **BASF. 1999. Determination of the Inhibition of Oxygen Consumption by Activated Sludge by Perylimid F in the Activated Sludge Respiration Inhibition Test according to GLP, EN 45001 and ICO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: March 1999). HERO ID: 4731542** | | | | | |
|---|---|---|---|---|---|---|
| **Note:** | Conducted according to OECD Guideline 209 | | | | | |
| **Domain** | **Metric** | **Qualitative Determination [*i.e.*, High, Medium, Low, Unacceptable, or Not rated]** | **Comments** | **Metric Score** | **Metric Weighting Factor** | **Weighted Score** |
| **Test Substance** | 1. Test substance identity | High | CAS, chemical name, production number and date, as well as the specific form of the test substance are all reported. | 1 | 2 | 2 |
| | 2. Test substance purity | High | Purity 98.9% reported by analysis | 1 | 1 | 1 |
| **Test Design** | 3. Study Controls | High | Blank Control was included and deviation of blank control was reported as <15%. A reference substance was also included. | 1 | 2 | 2 |
| | 4. Test Substance stability | High | Homogeneity, storage conditions, instability control were all reported and appeared to be appropriate for the test substance. | 1 | 1 | 1 |
| **Test Conditions** | 5. Test Method Suitability | Medium | Media concentrations were provided in terms of nominal concentrations (1000 mg/L) and were not measured. The reported limit of solubility (2800 mg/L) was not consistent with the limit of solubility of this chemical. | 2 | 1 | 2 |
| | 6. Testing Conditions | High | Testing conditions were recorded and were suitable for the test substance | 1 | 2 | 2 |
| | 7. Testing Consistency | High | Three blank controls, the test substance were conducted under the same conditions. | 1 | 1 | 1 |

| Study Reference: | BASF. 1999. Determination of the Inhibition of Oxygen Consumption by Activated Sludge by Perylimid F in the Activated Sludge Respiration Inhibition Test according to GLP, EN 45001 and ICO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: March 1999). HERO ID: 4731542 | | | | | |
|---|---|---|---|---|---|---|
| | 8. System Type and Design | Not Rated | This metric is not applicable as this is not an equilibrium test | NR | NR | NR |
| **Test Organisms** | 9. Test Organism Degradation | High | Inoculum source was a laboratory wastewater plant treating municipal and synthetic sewage; the dry substance concentration of the inoculum was reported as 1 g/L | 1 | 2 | 2 |
| | 10. Test Organism Partitioning | Not Rated | This metric is not applicable as this is not a partitioning study | NR | NR | NR |
| **Outcome Assessment** | 11. Outcome Assessment Methodology | High | The outcome assessment methodology is acceptable to determine the inhibition of oxygen consumption by activated sludge. | 1 | 1 | 1 |
| | 12. Sampling Methods | Medium | Sampling methods were not specifically discussed, but the results of daily analysis of the test variables were reported so this is not expected to impact the results of the test. | 2 | 1 | 2 |
| **Confounding/ Variable Control** | 13. Confounding Variables | High | One study group was used as this was conducted as a limit test. No confounding variables were observed or reported by the study authors. | 1 | 1 | 1 |
| | 14. Outcomes Unrelated to Exposure | High | Deviation of blank controls were reported to be <15%, which demonstrated the health of the test organism. | 1 | 1 | 1 |
| **Data Presentation and Analysis** | 15. Data Reporting | High | Study was conducted as a limit test, so no effects were observed in the study group. Study authors calculated and reported EC20, EC50, and EC80 of reference substance as well as the control. | 1 | 2 | 2 |

| Study Reference: | BASF. 1999. Determination of the Inhibition of Oxygen Consumption by Activated Sludge by Perylimid F in the Activated Sludge Respiration Inhibition Test according to GLP, EN 45001 and ICO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: March 1999). HERO ID: 4731542 | | | | | |
|---|---|---|---|---|---|---|
| | 16. Statistical Methods and Kinetic Calculations | Not Rated | Statistical analysis was not conducted as no adverse effects were reported. | NR | NR | NR |
| **Other** | 17. Verification or Plausibility of Results | High | Reported values were within expected range as defined by the reference substance, 3,5-dichlorophenol. | 1 | 1 | 1 |
| | 18. QSAR Models | Not Rated | QSAR models were not used as part of this study. *Note that this metric has been updated, as it was originally evaluated for a metric that is not part of the data quality criteria for fate data. | NR | NR | NR |
| | | | **Sum of scores:** | 16 | 19 | 21 |
| High | Medium | Low | **Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:** | 1.105 | **Overall Score (Rounded):** | 1.1 |
| ≥1 and <1.7 | ≥1.7 and <2.3 | ≥2.3 and ≤3 | | | **Overall Quality Level:** | High |

**Table 3. Biodegradability Study for C.I. Pigment Violet 29, BASF (1999a)**

| Study Reference: | BASF. 1999. Determination of the Biodegradability of Perylimid F in the Manometric Respirometry Test according to GLP, EN 45001 and ISO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: July 1999). HERO ID: 4731543 | | | | | |
|---|---|---|---|---|---|---|
| **Note:** | Conducted according to OECD Guideline 301F | | | | | |
| **Domain** | **Metric** | **Qualitative Determination [*i.e.*, High, Medium, Low, Unacceptable, or Not rated]** | **Comments** | **Metric Score** | **Metric Weighting Factor** | **Weighted Score** |
| **Test Substance** | 1. Test substance identity | High | CAS, chemical name, production number, state and date of production were all reported | 1 | 2 | 2 |
| | 2. Test substance purity | High | Purity reported as 98.9%. | 1 | 1 | 1 |
| **Test Design** | 3. Study Controls | High | Blank control and reference substance were included (Aniline); deviation and control chemical were acceptable according to test validity criteria of the guideline. | 1 | 2 | 2 |
| | 4. Test Substance stability | High | Homogeneity, storage conditions, instability controls were all reported. | 1 | 1 | 1 |
| **Test Conditions** | 5. Test Method Suitability | Medium | Media concentrations were provided in terms of nominal concentrations (100 mg/L) which was far higher than the limit of solubility. | 2 | 1 | 2 |
| | 6. Testing Conditions | High | Biodegradation values were measured and reported (28 days) according to reporting recommendations of Guideline. Test temperatures throughout the test were not explicitly reported, but the study authors indicated that the test was conduicted "at room temperature". | 1 | 2 | 2 |
| | 7. Testing Consistency | High | Five control samples and seven test samples were conducted under the same condition. | 1 | 1 | 1 |

| Study Reference: | BASF. 1999. Determination of the Biodegradability of Perylimid F in the Manometric Respirometry Test according to GLP, EN 45001 and ISO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: July 1999). HERO ID: 4731543 | | | | | |
|---|---|---|---|---|---|---|
| | 8. System Type and Design | Not Rated | Not an equilibrium test. | NR | NR | NR |
| **Test Organisms** | 9. Test Organism Degradation | High | Inoculum source reported as municipal activated sludge from laboratory wastewater treatment plants fed with municipal sewage which is appropriate. | 1 | 2 | 2 |
| | 10. Test Organism Partitioning | Not Rated | This is not a partitioning test. | NR | NR | NR |
| **Outcome Assessment** | 11. Outcome Assessment Methodology | High | The test methodology addressed the intended outcome of interest (biodegradation according to the parameters measured). | 1 | 1 | 1 |
| | 12. Sampling Methods | Medium | Sampling methods were not specifically discussed, but the results of daily analysis of the test variables were reported. | 2 | 1 | 2 |
| **Confounding/ Variable Control** | 13. Confounding Variables | Medium | The result (Measured BOD) of one blank sample deviated from other 6 test samples. The authors acknowledged and disregarded this sample. | 2 | 1 | 2 |
| | 14. Outcomes Unrelated to Exposure | Medium | 6 out of 7 test samples showed similar results, the degradation rate of all test samples did not show any inhibition from the test substance; One blank sample showed anomalous results discussed by the authors. The viability of organism was well maintained. | 2 | 1 | 2 |
| **Data Presentation and Analysis** | 15. Data Reporting | High | The study received a high rating for this metric | 1 | 2 | 2 |
| | 16. Statistical Methods and Kinetic Calculations | Medium | No statistical analyses were conducted; however, sufficient data were provided to conduct | 2 | 1 | 2 |

| Study Reference: | BASF. 1999. Determination of the Biodegradability of Perylimid F in the Manometric Respirometry Test according to GLP, EN 45001 and ISO 9002. Study conducted by BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056 Ludwigshafen (Study Completion Date: July 1999). HERO ID: 4731543 | | | | | |
|---|---|---|---|---|---|---|
| | | | an independent statistical analysis. | | | |
| **Other** | 17. Verification or Plausibility of Results | High | Reported values were within expected range as defined by reference substance(s); Aniline. | 1 | 1 | 1 |
| | 18. QSAR Models | Not Rated | QSAR models were not used as part of this study. | NR | NR | NR |
| | | | **Sum of scores:** | **20** | **20** | **25** |
| High | Medium | Low | **Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:** | 1.250 | **Overall Score (Rounded):** | 1.3 |
| ≥1 and <1.7 | ≥1.7 and <2.3 | ≥2.3 and ≤3 | | | **Overall Quality Level:** | High |

**References**


BASF. (1999a). Determination of the biodegradability of perylimid F in the manometric respirometry test according to GLP, EN 45001 and ISO 9002. Ludwigshafen: BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056.

BASF. (1999b). Determination of the inhibition of oxygen consumption by activated sludge by perylimid F in the activated sludge respiration inhibition test according to GLP, EN 45001 and ICO 9002. Ludwigshafen: BASF Aktiengesellschaft Ecology and Environmental Analytics Laboratory of Ecology D-67056.

U.S. EPA. (2012). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11 [Computer Program]. Washington, DC. Retrieved from https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

U.S. EPA. (2018). Application of systematic review in TSCA risk evaluations. (740-P1-8001). Washington, DC: U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention. https://www.epa.gov/sites/production/files/2018-06/documents/final_application_of_sr_in_tsca_05-31-18.pdf.